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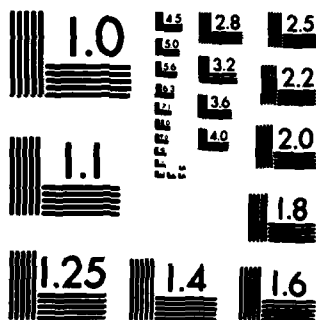
SPACE CHARGE INTERFACIAL KINETICS AND ELECTRICAL
RESPONSE OF CONDENSED MA. (U) NORTH CAROLINA UNIV AT
CHAPEL HILL DEPT OF PHYSICS AND ASTRON. J R MACDONALD
24 AUG 84 ARO-17996.12-CH DAAG29-81-K-0144 F/G 7/4

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) This final report describes the aims of the work, the personnel involved, and the main accomplishments of the research.		

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Space Charge, Interfacial Kinetics, and
Electrical Response of Condensed Matter

FINAL REPORT

J. Ross Macdonald

8/24/84

U.S. ARMY RESEARCH OFFICE

Contract No. DAAG29-81-K-0144

Department of Physics and Astronomy
University of North Carolina
Chapel Hill, N.C.



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I. Statement of the Problem Studied

The work of this contract was "particularly directed at understanding the interfacial processes which occur within the double layer and their relation to overall electrical response..."* The work proposed was "concerned with the electrical behavior of (ionic-conduction) systems in which a nonmetallic solid or liquid is in contact with metal electrodes or a concentrated electrolyte."*

The work was originally funded for 1 July 1981 through 30 June 1984. A no-cost extension was granted to 31 December 1984 and changed to 14 August 1984 upon receipt by the P.I. and his institution of a new A.R.O. contract beginning 15 August 1984. Thus this final report includes work done only through 14 August 1984.

II. Summary of Most Important Results

➤ The completed results of the work of this contract appear in the 12 papers of the enclosed publication list. Of particular importance is the work on lattice gas models of the double layer, (numbers 4, 7, 1P, and 2P, where P indicates papers in the pending publication list). Since the work has been described in some detail in earlier reports, such description will not be repeated here.

➤ It is, however, important to note that we are the first group to obtain significant results for systems involving dipoles of finite rather than infinitesimal length. (Papers 2, 5, 6, 8, 9, and 3P) ➤ Some of the

➤ papers are concerned one way or another with the interpretation of impedance data in dielectric and conductive systems involving

* Quotation from the original proposal.

liquid or solid state electrolytes. We believe that they have contributed appreciably to providing new and better ways to analyze and interpret small-signal ac data in these fields.

Not included on the publication list are three areas of work in progress which have not yet resulted in papers ready for publication. The first involves the preparation of a joint monograph on impedance spectroscopy. The present P.I. will be the principal editor, and during a three-months visit to Austria in the spring of 1984, he prepared first-drafts of several chapters (a total of about 130 pages). This work, in conjunction with other co-authors, will be continuing for some time. In addition, the P.I. has made appreciable progress on work on the small-signal frequency response of dielectric and/or conductive systems involving a distribution of activation energies - a common physical situation. A paper on this work should be completed soon. Finally, Dr. S. W. Kenkel has made substantial progress on the Monte Carlo analysis of the response of a monolayer of infinitesimal or finite-length dipoles under a static applied field. This work, important for the inner-layer region of the electrochemical double layer, takes almost all electrostatic interactions, planar and perpendicular, into account in an exact fashion. It is already showing results quite different from those of previous more approximate approaches.

Finally, it may be worth mentioning that parts of the work done under this contract have been presented as talks at scientific meetings, for example at: the Montreal, Canada meeting of the American Electrochemical Society, 1982; the Southeastern meeting of

the American Physical Society, 1983; and the 6th. Australian Conference on Electrochemistry, 1984.

We are most grateful for the continuing support of this work by the Army Research Office and for many helpful and pleasant interactions with A.R.O. Staff.

III. List of all Publications and Technical Reports Published.

This list is presented on page 4.

IV. List of Participating Scientific Personnel

Dr. J. R. Macdonald, P.I.

Dr. S. W. Kenkel, postdoctoral research associate

Mr. C. A. Hull, graduate student; earned M.S. degree on the project (part time).

Mr. G. B. Cook, undergraduate physics student (part time).

Mr. R. L. Hurt, undergraduate physics student (part time).

Contract No. DAAG 29-81-K-0144
(1 July 1981 - 15 August 1984)

Publications and Reports - Published

1. J. R. Macdonald, "Layered Lattice Gas Model for the Metal-Electrolyte Interface," *Surface Science* 116, 135-147 (1982).
2. S. W. Kenkel, G. Simons, and J. Hermanns, "On the Nearest Neighbor Separation of Finite Size Particles," *Molecular Physics* 47, 431-434 (1982).
3. J. R. Macdonald and D. R. Franceschetti, "Small-Signal A.C. Response Theory for Electrochromic Thin Films," *J. Electrochem. Soc.* 129, 1754-1756 (1982).
4. J. R. Macdonald and S. H. Liu, "An Iterated Three-Layer Model of the Double Layer with Permanent Dipoles," *Surface Science* 125, 653-678 (1983).
5. J. R. Macdonald and S. W. Kenkel, "Semi-empirical Expression for the Dielectric Constant of Polar, Polarizable Liquids," *J. Phys. D.: Appl. Phys.* 16, L195-L198 (1983).
6. J. R. Macdonald and C. A. Hull, "Pseudo Reaction Rate in the AC Response of an Electrolytic Cell," *J. Electroanal. Chem.* 165, 9-20 (1984).
7. J. R. Macdonald and S. W. Kenkel, "A Finite-Length-Dipole Model of the Double Layer in Polar, Polarizable Materials," *J. Chem. Phys.* 80, 2168-2182 (1984).
8. J. R. Macdonald, "Note on the Parameterization of the Constant-Phase Admittance Element," *Solid State Ionics* 13, 147-149 (1984).
9. J. R. Macdonald and G. B. Cook, "Analysis of Impedance Data for Single Crystal Na β -Alumina at Low Temperatures," *J. Electroanal. Chem.* 168, 335-354 (1984).

Publication and Reports - Pending Publication

1. S. W. Kenkel, "Monte Carlo Simulation of a Lattice Gas Model of the Electrical Double Layer," submitted to *Molecular Physics*.
2. S. W. Kenkel and J. R. Macdonald, "A Lattice Model for the Electrical Double Layer Using Finite-Length Dipoles," accepted by *J. Chem. Phys.*
3. S. W. Kenkel, "A Simple Closed-Form Approximation for the Williams-Watts Dielectric Response Function," submitted to *J. Appl. Phys. D.*

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